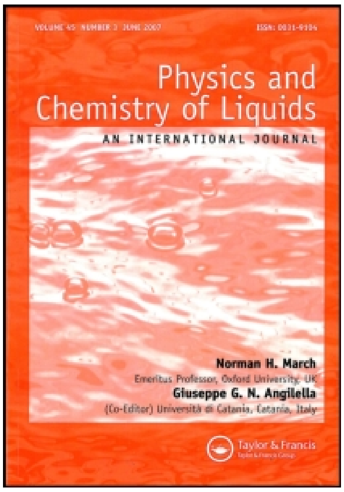

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Vapour–liquid equilibria of the binary mixtures of some aliphatic alcohols and chloroethanes or chloroethylenes

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Bubble temperatures at 95 kPa, over the entire composition range are measured for the binary mixtures: *iso*-propanol + 1,1,1-trichloroethane, +1,1,2,2-tetrachloroethane and +tetrachloroethylene and trichloroethylene + methanol, and +*n*-propanol and +*n*-butanol – using a Swietoslawski-type ebulliometer. The liquid composition *versus* bubble temperature measurements are found to be well represented by the Wilson model and the resulting vapour–liquid equilibrium information is reported.

Keywords: Vapour–liquid equilibria; Bubble temperatures; Aliphatic alcohols; Chlorohydrocarbons

1. Introduction

This investigation on the vapour–liquid equilibria of the binary mixtures noted in the abstract is a continuation of our recent studies on the phase equilibria of the binary mixtures containing chlorohydrocarbons and alcohols [1–4]. The measurements have been carried at 95 kPa. Among the mixtures chosen for the present study, the methanol (1) + trichloroethylene (2) system has been investigated by Firzweiler and Dietrich [5] while the trichloroethylene (1) + *n*-propanol (2) has been studied at 101.3 kPa by Sagnes and Sanchez [6] and Venkateswara Rao and Chiranjivi [7] and at 20 and 100 kPa by Aucejo *et al.* [8]. The trichloroethylene (1) + *n*-butanol (2) system has been studied at 101.3 kPa by Raviprasad *et al.* [9] and at 20 and 100 kPa by Deoz *et al.* [10]. We could not locate any experimental data on the other systems chosen for this study in the open literature.

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2. Experimental section

2.1 *Method*

A Swietosawski-type ebulliometer, very similar to the one described by Hala *et al.* [11], has been used for the present experimental investigation. Connection of the ebulliometer to a good vacuum system and dry nitrogen gas cylinder, through a mercury manometer in line, facilitated the creation and the maintenance of the chosen pressure within ±1 mm Hg. The equilibrium temperatures are measured to an accuracy of $\pm 0.1^\circ$C by means of a platinum resistance thermometer, carefully calibrated by means of point-to-point comparison with a Standard Platinum Resistance Thermometer certified by the National Bureau of Standards, Boulder (USA). The liquid mixtures for the studies are prepared gravimetrically, making use of an electronic balance precise to ±0.0001 g and stirred well before being placed in the ebulliometer. The heating rate is adjusted to result in the desired condensate drop rate of 30 drops per minute in accordance with the suggestion of Hala *et al.* [11]. The equilibrium temperatures, measured after the steady drop rate and constancy of temperature are maintained for at least 30 min, are reported.

2.2 *Materials*

AR grade chemicals used in this study are further purified according to the easiest possible method described in [12]. Purity of the chemicals is ascertained by measuring the density and refractive index, which compare favourably with the literature values as shown in table 1.

3. Results and discussion

The experimental liquid phase composition (x_1) *versus* temperature (T) data, summarized in table 2, are fitted to the Wilson [13] model. The optimum Wilson parameters are obtained by minimizing the objective function defined as

$$\varphi = \sum [(P_{\text{cal}}/P_{\text{expt}}) - 1]^2 \tag{1}$$

Table 1. Comparison of the density (D) and refractive index (n) of the pure substances used in this study with literature data from Riddick *et al.* [12] at 298.15 K.

	D (kg/m^{-3})		n	
Substance	This work	Riddick *et al.* [12]	This work	Riddick *et al.* [12]
Methanol	791.1	791.10	1.3287	1.32872
n-Propanol	804.1	804.00	1.3855	1.38556
iso-Propanol	781.3	781.26	1.3752	1.37520
n-Butanol	811.1	811.00	1.3993	1.39929
1,1,1-Trichloroethane	1329.9	1329.90	1.4359	1.43590
1,1,2,2-Tetrachloroethane	1586.7	1586.66	1.4914	1.49140
Trichloroethane	1462.0	1462.00	1.4765	1.47469
Tetrachloroethylene	1614.3	1614.32	1.5032	1.50320

Table 2. Vapor–liquid equilibria of selected binary mixtures of *iso*-propanol + chlorohydrocarbons and trichloroethylene + aliphatic alcohols at 95 kPa.

1,1,1-Trichloroethylene (1) + isopropanol (2)			*iso*-Propanol (1) + 1,1,2,2-tetrachloroethane (2)			*iso*-Propanol (1) + tetrachloroethylene (2)		
x_1	T/K	y_1	x_1	T/K	y_1	x_1	T/K	y_1
0.0000	353.85	0.0000	0.0000	407.05	0.0000	0.0000	391.85	0.0000
0.1411	348.65	0.2976	0.1260	386.15	0.6431	0.1811	360.05	0.6686
0.2632	345.95	0.4449	0.2240	376.75	0.7630	0.2512	358.25	0.6940
0.4321	343.65	0.5735	0.3020	371.95	0.8145	0.3071	357.55	0.7085
0.6120	342.25	0.6700	0.4190	367.05	0.8637	0.4410	356.15	0.7366
0.7613	342.05	0.7473	0.5650	362.75	0.9046	0.5212	355.55	0.7535
0.8713	342.85	0.8233	0.7420	358.75	0.9433	0.6112	354.85	0.7754
0.9322	343.85	0.8861	0.8280	356.05	0.9612	0.7312	354.35	0.8138
1.0000	345.25	1.0000	0.9350	354.05	0.9845	0.8110	354.05	0.8485
			1.0000	353.85	1.0000	0.8912	353.95	0.8969
						1.0000	353.85	1.0000

Methanol (1) + trichloroethylene (2)			Trichloroethylene (1) + *n*-propanol			Trichloroethylene (1) + *n*-butanol (2)		
x_1	T/K	y_1	x_1	T/K	y_1	x_1	T/K	y_1
0.0000	357.55	0.0000	0.0000	368.65	0.0000	0.0000	388.05	0.0000
0.1058	334.95	0.5581	0.1447	360.15	0.3748	0.1518	371.95	0.5493
0.1500	333.35	0.5878	0.2990	355.85	0.5414	0.3030	364.65	0.7062
0.3057	331.55	0.6270	0.4545	353.75	0.6291	0.4537	361.25	0.7759
0.4453	331.05	0.6432	0.6068	352.85	0.6857	0.6037	359.15	0.8184
0.5961	330.75	0.6616	0.7470	352.65	0.7331	0.7530	357.85	0.8557
0.7562	330.75	0.6970	0.8936	353.45	0.8113	0.9016	357.15	0.9115
0.8543	331.15	0.7449	0.9765	355.15	0.9292	1.0000	357.55	1.0000
0.9014	332.10	0.7865	1.0000	357.55	1.0000			
1.0000	336.05	1.0000						

Table 3. Antoine constants for the equation $\ln(P/\text{kPa}) = A - B/[(T/\text{K}) + C]$.

Substance	A	B	C
Methanol	16.5726	3626.55	− 34.30
n-Propanol	15.5289	3166.37	− 80.20
iso-Propanol	16.6755	3640.20	− 53.54
n-Butanol	15.2009	3137.01	− 94.40
1,1,1-Trichloroethane	13.9897	2802.75	− 48.15
1,1,2,2-Tetrachloroethane	14.0633	3341.88	− 62.15
Trichloroethylene	14.1678	3023.13	− 43.20
Tetrachloroethylene	14.1468	3259.27	− 52.15

where P_{cal} and P_{expt} stand for the calculated and experimental total pressures. The Nelder–Mead optimization technique described by Kuester and Mize [14] has been used. Saturated vapour pressures of the pure liquids, needed in the computations are calculated from the Antoine constants collected from the literature and noted in table 3, for ready reference. The Antoine equation, with the constants noted in table 3, represents the literature vapour pressure data as well as the present measurements with an average absolute deviation of 0.5%, for all the pure liquids of the present study. The molar volumes of the pure liquids, calculated from the density measurements of this study (recorded in table 1) are used as the input in obtaining the optimum Wilson parameters. The vapour phase mole fractions predicted from

Table 4. Representation of the measurements by Wilson model.

Mixture	$[(\lambda_{12}-\lambda_{11})/R]/K$	$[(\lambda_{12}-\lambda_{22})/R]/K$	Std. Dev. in T/K
1,1,1-Trichloroethane (1) + *iso*-propanol (2)	64.39	347.42	0.12
iso-Propanol (1) + 1,1,2,2-tetrachloroethane (2)	110.27	141.50	0.03
iso-Propanol (1) + tetrachloroethylene (2)	596.18	219.30	0.12
Methanol (1) + trichloroethylene (2)	692.97	425.74	0.05
Trichloroethylene (1) + *n*-propanol (2)	126.92	522.32	0.03
Trichloroethylene (1) + *n*-butanol	161.80	463.71	0.03

Table 5. Summary of comparisons with literature data.

Source of literature data	Condition	Av. abs. deviation in y_1
Methanol (1) + trichloroethylene (2) mixture		
Fritzweiler and Dietrich [5]	760 mm Hg	0.012
Trichloroethylene (1) + n-propanol (2) mixture		
Sagnes and Sanchez [6]	760 mm Hg	0.013
Venkateswara Rao and Chiranjivi [7]	760 mm Hg	0.016
Aucejo *et al.* [8]	150 and 750 mm Hg	0.008
Trichloroethylene (1) + n-butanol(2) mixture		
Raviprasad *et al.* [9]	760 mm Hg	0.035
Doez *et al.* [10]	150 and 750 mm Hg	0.007

the Wilson model are also given in table 2. Results of the representation of the phase equilibrium data by the Wilson [13] model, summarized in table 4, indicate that the data and the representation are quite good. Comparisons of the vapour phase mole fractions calculated from the Wilson constants derived from the present work (noted in table 4) with the experimental observations of the earlier investigators are summarized in table 5. The agreement on the whole is satisfactory. The data and the representation presented in the article are expected to be useful for engineering design purposes.

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